

N,N-Diethylaniline
91-66-7 | DTXSID8021800

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 205 °C

Global applicability domain: Inside

Local applicability domain index: 6.57e-01

Confidence level: 8.44e-01

Nearest Neighbors from the Training Set

Image not found

N,N-Diethylaniline

Measured: 216

Predicted: 205

Image not found

Benzenamine, N,N,2,6-tetramethyl-

Measured: 196

Predicted: 204

Image not found

Benzenamine, N-ethyl-N-methyl-

Measured: 204

Predicted: 201

Image not found

N,N,2-Trimethylaniline

Measured: 194

Predicted: 201

Image not found

N,N,4-Trimethylaniline

Measured: 211

Predicted: 201